# REPORT DOCUMENTATION PAGE

Form Approved OMB No. 0704-0188



| 1. REPORT DATE *(DD-MM-YYYY)* | 2. REPORT TYPE | 3. DATES COVERED *(From – To)* |
|---|---|---|
| 24-07-2002 | Conference Proceedings | 15 July 2001 - 20 July 2001 |

**4. TITLE AND SUBTITLE**

Workshop on Atomistic-to-Continuum Models or Long molecules and Thin Films

**5a. CONTRACT NUMBER**
F61775-01-WF071

**5b. GRANT NUMBER**

**5c. PROGRAM ELEMENT NUMBER**

**6. AUTHOR(S)**

Conference Committee

**5d. PROJECT NUMBER**

**5d. TASK NUMBER**

**5e. WORK UNIT NUMBER**

**7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)**

Ecole Polytechnique Federale de Lausanne
MA Ecublens
Lausanne CH-1015
Switzerland

**8. PERFORMING ORGANIZATION REPORT NUMBER**

N/A

**9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)**

EOARD
PSC 802 BOX 14
FPO 09499-0014

**10. SPONSOR/MONITOR'S ACRONYM(S)**

**11. SPONSOR/MONITOR'S REPORT NUMBER(S)**
CSP 01-5071

**12. DISTRIBUTION/AVAILABILITY STATEMENT**

Approved for public release; distribution is unlimited.

**13. SUPPLEMENTARY NOTES**

20040625 087

**14. ABSTRACT**

The Final Proceedings for Workshop on Atomistic-to-Continuum Models or Long molecules and Thin Films, 15 July 2001 - 20 July 2001

This is an interdisciplinary conference. Topics include long thin molecules,wide thin films, and the role and theory of rapid oscillations and constraints.
In each area the speakers will be divided between those whose background is primarily in Molecular Dynamics and Atomistic Models, and those whose background is primarily Continuum Mechanics and Mathematics

**15. SUBJECT TERMS**

EOARD, Polymer Chemistry, Molecular Design, Computational Mathematics, Mathematical Modeling

| 16. SECURITY CLASSIFICATION OF: | | | 17. LIMITATION OF ABSTRACT | 18, NUMBER OF PAGES | 19a. NAME OF RESPONSIBLE PERSON |
|---|---|---|---|---|---|
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# Report on the Workshop on
# Atomistic to Continuum Models for Long Molecules and Thin Films

**Center Stefano Franscini**
**Monte Verita, Ascona, Switzerland**

**July 15--20 2001**

The objective of this one-week long workshop was to bring experts from around the world together for intensive discussions addressing mathematical and computational issues arising in bridging the gaps in length and time scales between atomistic descriptions and reduced-order continuum mechanics models of scientifically and technologically important molecular systems. The conference focussed on systems that have both a small and a long length scale. Examples are long stiff polymers such as DNA, and thin films of only a few atoms thickness, but with a large extent.

In addition to funds received directly from the Mte Verita Conference Centre itself, the conference was sponsored by the European Office of Aerospace Research and Development, Office of Naval Research International Field Office, Compaq, the European Science Foundation - Programme SIMU, and the Department of Mathematics, Swiss Federal Institute of Technology Lausanne.

There were a total of 50 attendees from 8 countries, with 19 talks and 11 posters. Full poster titles and talk titles and abstracts are available at the web page:

http://lcvmwww.epfl.ch/~lcvm/ascona2001/index.html

Independently, in Attachment A there is appended a listing of all talk titles and abstracts, along with a list of attendees with full addresses. In addition, in Attachment B there is provided a written summary of all the talks that was prepared by a Rapporteur (Dr. M. Moakher).

Overall the conference was judged to be a great success according to the comments received from the participants. In particular many participants felt that the major strength of the meeting was the truly interdisciplinary character with a small overall attendance, and within a completely residential setting. This meant that practitioners coming from the fields of mathematics, mechanics, physics, chemistry and biology had the opportunity not only to listen to talks from scientists in the other fields, but also to follow up with informal discussions, and thus to obtain a meaningful entree into the literature and approaches of the other disciplines to the common problem of multi-scale modelling of atomistic systems.

One rather specific consequence of the meeting has been the establishment of the Ascona B-DNA Consortium (or ABC project http://apex.ibpc.fr/ABC/ ) This project is a consortium of Laboratories around the world who have agreed to pool computational resources in order to be able to construct a database of Molecular Dynamics simulations that will provide a compatible source of predictions of B-form DNA structural parameters as a function of all possible

tetramers within the sequence. One possible use of such a database is in the construction of mesoscopic models of DNA fragments.

## Attachment B Summary of all talks

**Rapporteur: Dr. M. Moakher**

The participants of this workshop come essentially from two different backgrounds: molecular biology and computational chemistry, and continuum physics and mathematics. Because of the interdisciplinary nature of the workshop, speakers were asked to be as clear as possible and to adapt to the flow of questions raised by the audience during the presentation.

Most of the talks put an emphasis on the role of the mesoscale in the effort to bridge the gap between micro and macro scales. Among the terms that were mentioned frequently during the workshop were degrees of freedom thinning/reduction, coarse graining, full resolution atomistic description, reduced-order continuum models. In what follows, a summary is given of the talks in chronological order during the workshop.

Prof. D. Beveridge gave an overview talk about the structure of DNA and discussed experimental and computational methods for measuring DNA bending. MD simulation history was presented and current issues were discussed. The main points of this talk were the need to develop sequence-dependent models that take into account the effects of environment (counter ions), the study of the wide spectrum of models from high-resolution all atoms to reduced-order continuum models and the necessity to validate MD simulations

Prof. R. Phillips presented recent work on systematic ways of degrees of freedom thinning for 2D model proteins, $\alpha$-helices and $\beta$-sheets. This approach has been successful in some material science problems. The message of this talk was to search for structural motifs and to use kinematic constraints in order to reduce some degrees of freedom. Full atomistic resolution is not needed for the whole structure.

Dr. O. Gonzalez reviewed rigid base-pair and continuum rod models of DNA. He presented a method, consistent with equilibrium statistical mechanics, for extracting a complete set of parameters for the rigid base-pair model from a time series of MD simulations. The corresponding parameters for the elastic rod were given. The summary of this talk was that there are rational ways to bridge the gap between all-atom MD simulations and reduced-order models, but these methods are not unique and depend on the assumptions made.

Prof. T. R. Powers discussed the mechanics of flagellar systems for bacteria such as E. Coli and Salmonella. The elements of bacterial motility are elasticity and drag, polymorphism, and hydrodynamic interactions.The bundling of rotating helical flagella arises from two distinct effects: the counter rotation of the cell body, and the swirling flows set up by each individual flagellum.

Dr. Lankas talked about how he used MD simulations to obtain the local and global mechanical properties of oligomers. He stressed the fact that different definitions of the total length of an oligomer can lead to different global bendability coefficients.

Prof. R. Tuzun described the normal coordinate analysis method used for large chemical systems. This method requires diagonalization of the Hessian matrix. Non-physical negative eigenvalues obtained numerically can be eliminated by averaging the Hessian matrices over a trajectory of an MD simulations. Also, he pointed out that approximate methods not requiring full diagonalization yield little change in the computed thermodynamic properties but save computational effort.

Prof. A. DeSimone talked about soft elastic response of nematic elastomers. By quasi-convexification of the microscopic energy, explicit solutions and a phase diagram were obtained. He stressed the role of the mesoscale in the process of degrees of freedom thinning when one passes from micro to macro scales. The collective behavior of the microstructure is complex yet yields understandable response.

Dr. S. Reich showed in his talk how smoothed particle hydrodynamics yield Newtonian equations of motion similar in structure to those used in MD simulations. The point of his talk was that methods of fluid dynamics could be quite useful in MD simulations.

Dr. F. Mueller-Plathe talked about the multiscale approach to polymer simulations in melt and in solutions. This approach is a valuable tool in many engineering applications and provides a link to standard engineering simulations such as FEM. However, this method is non-standard and needs further development.

Prof. R. Osman discussed the role of flexibility in damage recognition and repair enzymes efficiency. He stressed the fact that DNA is important only in the presence of proteins. The interaction of proteins with DNA leads to changes in environment, structure and dynamics. He pointed out that full atomistic representation of the interaction is not practical and mesoscopic representation is very much needed.

Dr. A. Gusev presented a finite-element based approach for obtaining effective properties of three-phase materials. The use of periodic morphology and adaptative unstructured meshes yield accurate prediction of the behavior of multi-phase materials.

Prof. G. Friesecke talked about coarse graining for some elasticity problems. In particular, he discussed the thin plate limit of a 3D elastic body and the modeling of Carbon nanotubes. The message of this talk is that it is possible to eliminate degrees of freedom by rigorous analysis of certain problems knowing only the governing equations.

Prof. H. Berendsen was asked by Dr. R. Lavery to give the ``big picture" of the state of computational chemistry. After giving an overview of the computational chemistry of the 20th century, he stated that {\it ab initio} simulations of complex molecular systems will be the subject of computational chemistry in the 21st century. The message of this talk was that mathematicians should be aware, when making simplifications, of the requirement of statistical mechanics and the relations to thermodynamic quantities. A bottleneck of computational chemistry will be the incorporation of quantum dynamics into classical dynamics. He concluded his talk by suggesting that some physics, chemistry and biology should be included in the education of mathematician and that more mathematics should be incorporated into the education of chemists and biologists.

Prof. H. Sklenar presented a Monte Carlo Metropolis algorithm for sampling the conformational dynamics of nucleic acids. The conclusion of his talk was that with an improvement of solvent electrostatic forces this algorithm could become an alternative to conventional MD simulations.

Dr. S. Conti talked about debonding and blistering of thin films. He explained the folding perpendicular to the debonded region by minimization of the elastic energy used in F\"oppl-van K\'arm\'an theory of plates. He showed that this plate model is equivalent to the full 3D elasticity theory.

Dr. M. Kroeger presented recent advances in the modeling of polymer melts, wormlike micella, and branched systems at microscopic scales. He discussed the validity of Fokker-Planck description using nonequilibrium MD and experimental results.

Prof. M. Parrinello showed how {\it ab initio} molecular dynamics can take environment effects into account. He presented a method that has the promises of solving the limiting factor of time scale when simulating chemical reactions and processes.

Prof. R. James was asked by Prof. J. Maddocks to give a talk on the mathematical perspectives of coarse graining and averaging. He pointed out that multiscale mathematical methods need to be developed for going from atomistic description to continuum description. The lack of available methods that give the continuum description from MD simulations urges chemists and physicists to profit from weak convergence results and use it in developing creative algorithms. Similarly, mathematicians should use the ideas of weak convergence to formulate new concepts for computations.

Dr. W. Huisinga presented in his talk a general technique for analyzing metastability of Markovian systems. The method he presented can be used to derive reduced models by identification of the essential degrees of freedom and to enhance Monte Carlo sampling methods.

Dr. K. Klenin presented a Brownian dynamic approach to intrachain chemical reaction of supercoiled DNA. His method extends to intermediate reaction rates earlier studies that are valid for slow and fast reaction rates. He showed that collisions by reptation and collisions by reptation have different reaction times.

Prof. H. Berendsen presented methods to speed up molecular dynamics simulations by use of tricks and the identification of a reaction coordinate along which motion is slow. The point of his talk is that most biological rate processes are strongly damped barrier-crossing processes for which the Smoluchowski limit is valid.